Unveiling how ventilated packaging design and cold chain scenarios affect the cooling kinetics and fruit quality for each single citrus fruit in an entire pallet

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Abstract

Optimizing fresh fruit supply chains is essential to reduce food losses and the associated environmental impact, as large amounts of energy and natural resources are embodied in these lost products. Proper refrigeration of these perishable items is essential here, and the used ventilated packaging design and cold chain scenario play a key role. This study pioneers in unveiling how package design, package position on a pallet, package stacking pattern and cold chain scenarios affect the cooling kinetics and fruit quality evolution for every single fruit of the thousands of fruit inside a pallet. This enables us to identify fruit quality heterogeneities on a pallet level, where previous studies focused on an order of magnitude less fruit. For this purpose, our recently developed virtual cold chain methodology is applied to these large ensembles of fruit, which relies on computational fluid dynamics simulations. Of the three evaluated packaging designs for citrus fruit, the Supervent package outperforms the Standard and Opentop packaging by providing the overall fastest and most uniform cooling. Supervent's performance is attributed to the alignment of ventilation pathways through the lateral vent holes. The performance of the Standard package is very similar, apart from the inefficient cooling at lower speeds. The Opentop packaging exhibits lengthy and non-uniform citrus fruit cooling, due to the unequal distribution of the vent openings on its long and short sides, and near the top surface. This unequal distribution fosters the creation of preferential pathways and faster cooling of the top layer of fruit. Concerning the cold chain scenarios, forced-airflow precooling can bring down the temperature the fastest after harvest. The promising scenario "ambient loading", where citrus fruit are loaded at ambient temperatures in the container, proves to be a worthy alternative. We could also show that stacking the pallet in a mechanically more stable way negatively affects the cooling heterogeneity. Finally, our methodology enables us to identify for a certain cold chain, which box on the pallet the customer should choose to have the longest shelf life, or which box the retailer should sell first.

Keywords

virtual cold chain; citrus fruit; CFD; OpenFOAM; fruit quality; cooling

1. Introduction

Temperature is a key environmental parameter that affects the shelf life of fresh fruit and vegetables. A reduction of 10°C in fruit temperature typically doubles the shelf life because the product's metabolism and the associated deteriorative reactions are slowed down (Robertson, 2016; Thompson, 2004). As such, cooling of fresh produce after they are harvested, by removing the stored heat, and keeping these products cool throughout the cold chain are paramount for maximizing shelf life. Maintaining a low temperature, once the produce is cooled down, might seem trivial but is quite challenging in commercial cold chains. One reason is that the produce is usually exposed to elevated temperatures when it is transferred from one unit operation to another, for example during loading into a refrigerated container from the precooling facility. Product temperatures also rise during defrosting cycles in refrigerated containers or cold stores or during failure of the cooling system due to power outages. In addition to the initial precooling, produce thus often has to be partially recooled several times throughout its cold chain journey in different facilities. Fast and homogeneous (re)cooling of the fruit at different locations in each pallet of the cargo is therefore essential to minimize quality loss. By achieving an efficient cold chain: (1) food losses are reduced (Gardas, Raut, & Narkhede, 2018); (2) the spatial radius to market the produce is enlarged; (3) lengthier, but more environmentally-friendly, means of transport can be used, for example ship transport instead of airfreight; or (5) customers can keep the fruit longer fresh at home before consumption. The large impact of cooling on food losses (Arias Bustos & Moors, 2018; Gokarn & Kuthambalayan, 2017) also directly links to the environmental impact of food cold chains: for every fruit that is lost along the supply chain, the energy used in pre- and postharvest practices is indirectly lost as well (Fiore et al., 2018; Vinyes et al., 2017). Hence reducing these losses is essential for any sustainable fresh fruit industry.

The ventilated packaging in which fruit or vegetables are packed play a key role in how fast produce can be

(re)cooled, and how uniform this process is within, for example, a pallet of packed produce (Defraeye, Cronjé, Berry, et al., 2015; Galić, Ščetar, & Kurek, 2011; Opara & Mditshwa, 2013). Ventilated cartons or plastic crates are typically used for fresh produce (Opara & Mditshwa, 2013; Watkins, 2002; WPO, 2008). The cooling kinetics depend on the box dimension, the total vent area, the position of the vent holes and their shape, amongst others (Pathare, Opara, Vigneault, Delele, & Al-Said, 2012). Apart from the individual package design, also their stacking on the pallet plays a role as often a part of the vent holes are blocked. Finally, the (re)cooling efficacy of the package design is also closely related to the specific unit operation. Forced airflow cooling implies horizontal airflow at high flow rates (~ 1 L s^{-1} kg^{-1} (Brosnan & Sun, 2001; Thompson, 2008, 2004)) whereas in refrigerated containers vertical airflow is present with much lower airflow rates (0.02-0.06 L s^{-1} kg^{-1} (Defraeye, Cronjé, Verboven, Opara, & Nicolai, 2015)). Packaging also plays a key role in the environmental impact of refrigerated supply chains. Differences in environmental impact between ventilated packaging designs have been identified recently (Defraeye et al., 2016). Typical life-cycle assessment (LCA) however rarely incorporates the energy and fruit quality gains from better packaging systems (Wikström, Williams, Verghese, & Clune, 2014). In a recent study (Wu, Beretta, Cronje, Hellweg, & Defraeye, 2019), life-cycle assessment was performed to evaluate the environmental impact of different packaging designs, where significant differences were identified between ventilated carton designs. These differences in fruit quality evolution between different packaging designs are expected to become particularly pronounced for very perishable species (e.g. berries).

As packaging is so important in postharvest cold chains, a lot of valuable research was performed on the relation of package design to fruit cooling (Berry, Fadiji, Defraeye, & Opara, 2017; Defraeye et al., 2013; Dehghannya, Ngadi, & Vigneault, 2011, 2012; Ferrua & Singh, 2009; Pathare et al., 2012). Focus areas were, amongst others, the number, shape or position of vent holes, the total open area of the packaging, the impact of internal packaging (plastic liners, trays) and the occurrence of airflow bypass (Thijs Defraeye, Cronjé, Berry,

et al., 2015). These studies relied on both experimental and simulation-based techniques. Experiments are instrumental in measuring the temperature history of individual produce or airspeeds at specific positions inside the ventilated cartons. Setting up such experiments is, however, quite time consuming, particularly when large amounts of cartons, filled with fruit, have to be monitored. At most, only a few tens of fruit are typically monitored. Computational fluid dynamics (CFD) simulations, where every individual fruit can be modeled explicitly, are the preferred choice for a precise evaluation of the fruit cooling heterogeneity and airflow field inside the package (Ambaw et al., 2013; Dehghannya, Ngadi, & Vigneault, 2010; Norton & Sun, 2006; Norton, Tiwari, & Sun, 2013; Smale, Moureh, & Cortella, 2006; Wang & Sun, 2003). This explicit approach avoids the need for parameterized porous media approximations but entails a high computational cost. Thereby, CFD has only been applied to a single box or a few boxes of fruit, so typically for a few 100 fruits. The differences in airflow rates and airflow directions between the various unit operations, however, require that larger entities of packages are assessed together to provide an outcome on the cooling uniformity throughout the cargo. In a recent study, an entire pallet of fruit, where each fruit was explicitly modeled, was evaluated for the first time with CFD for one single package design (Wu & Defraeye, 2018). Clear non-uniform cooling between individual packages in each pallet was identified. As a next step, we identify how package design, its positioning on a pallet, package stacking pattern but also cold chain scenario affect the remaining fruit storage life of a complete pallet of fruit, and the related heterogeneities within the pallet. Answering these questions will give insight in how to improve ventilated packaging designs and cold chain scenarios to provide a longer and more uniform storage life of our fruit. Such comparisons between packaging designs and stacking patterns on pallets are especially of interest for the postharvest industry, including packhouses, precooling facility managers, exporters and importers of fresh produce but also R&D researchers and container manufacturers. For this purpose, the recently developed virtual cold chain (VCC) method is used (Wu et al., 2018), which relies on CFD simulations. As a case study, we target corrugated fiberboard cartons filled with orange fruit, stacked on a high-cube pallet. Three packaging designs of

ventilated cardboard boxes are evaluated concerning cooling performance for three subsequent unit operations in the refrigerated supply chain, namely forced airflow (pre)cooling, refrigerated container transport and cold storage. Also, three cold chain scenarios are considered. Here, also a prediction of the evolution of temperature-dependent fruit quality is included. Finally, the impact of the stacking pattern of the packages on a pallet is investigated. Identifying the cooling and quality heterogeneities between individual fruit on a pallet level was not done for different packaging and cold chain scenarios to our best knowledge.

2. Materials and methods

2.1. Virtual cold chain method

The virtual cold chain method was developed by (Wu et al., 2018). This method is actually a CFD-based workflow to obtain the thermal history as well as quality evolution of every individual fruit inside ventilated packaging throughout its entire cold chain (Figure 1). In the present study, an entire pallet of fruit is targeted. First, a computational model is built for a pallet for each of the unit operations (precooling, refrigerated transport, cold storage). Afterward, CFD simulations, calculating airflow and heat transfer, are performed for each unit operation. The thermal state of each fruit is transferred from one (virtual) unit operation (e.g., precooling) to the following one (e.g., transport) for each of the investigated cold chain scenarios. In that way, the cooling behavior is simulated throughout the entire virtual cold chain. Finally, a temperature-dependent kinetic rate-law is modeled to calculate the evolution of fruit quality of every single fruit, based on its simulated temperature history.

The VCC method relies on CFD as the main pillar for estimating fruit quality evolution. This computational engineering tool is commonly-used in research, R&D and industrial practice for process optimization, including

for making processes more green and sustainable (Azizi, Keshavarz, & Hassanzadeh, 2018; Ebrahimi-moghadam, Farzaneh-gord, Arabkoohsar, & Jabari, 2018; Wu et al., 2019; Xiao, Fu, Zhu, & Zhang, 2019; Zhang et al., 2018). In this study, an entire pallet of fruit is considered, where each fruit is modeled discretely with CFD. This implies an exceptionally large computational effort. As such, this amount of fruit is representative for industrial practice at a commercial scale, and can capture the thermal heterogeneity found in real pallets of fruit.

2.2. Packaging and palletization

Three different package designs are evaluated, namely Standard, Supervent and Opentop (Figure 2). The Standard and Supervent cartons are filled with 64 orange fruit (so 13.57 kg) and each Opentop carton is filled with 60 fruit (so 12.72 kg). All fruit are placed in the carton according to a staggered pattern. The citrus fruit are modeled explicitly by representing them as spheres (diameter 75 mm). The total open area (TOA) for each carton is specified in Table 1.

The Standard and Supervent boxes are stacked to assemble a high-cube pallet (1.2 m x 1.0 m x 2.16 m) containing 80 cartons and holding 5120 fruit (Figure 3). In total, 8 layers are stacked regularly on top of one another, where each layer contains 10 cartons. In total, 3 rows are present (Row1, Row2 and Row3) along the horizontal flow path for precooling and cold storage, and 8 layers (L1-L8) are present along the vertical flow path for refrigerated container transport. Each layer contains 10 cartons (C01-C10). For each layer, Row1 and Row2, respectively, have 3 cartons, whereas Row3 has 4 cartons (Figure 3).

For the Opentop boxes, 65 cartons are stacked to assemble a high-cube pallet (1.2 m x 1.0 m x 2.21 m) (Figure 3), which holds 3900 fruit. In total, 13 layers are stacked regularly on top of one another, and each layer

contains 5 cartons. This results in 2-3 rows (Row1, Row2 and Row3) along the horizontal flow pathway for precooling and cold storage, and 13 layers (L1-L13) along the vertical flow pathway for refrigerated container transport. Each layer contains 5 cartons (C01-C05). Note that Opentop cartons are precooled with airflow perpendicular to their short side (1 m wide) of the pallet (1 x 1.2 m), whereas Standard and Supervent cartons are precooled with airflow perpendicular to their long side (1.2 m wide). The main reason is that this helps to counteract for the reduced fruit stacking density for Opentop packaging. This reduced density implies that less fruit can be packed in the same pallet volume, due to their less dense stacking in the Opentop package. By positioning and cooling the pallet along its short side in the precooler, more Opentop pallets can be placed in one precooling room, so a larger amount of fruit can be cooled simultaneously. Even in this case, the resulting stacking density for a single pallet is lower than for Supervent.

In addition to the regular 8-layers stacking of the Supervent cartons, staggered stacking is also evaluated (Figure 4) as this can provide additional stability of the pallet. This configuration however blocks a part of the vertical vent holes and thereby some of the vertical ventilation pathways. By comparing both stacking patterns, we aim to evaluate how the cooling rate is affected by this more stable alternative.

2.3. Computational model

The cold chain involves three different unit operations, namely precooling, refrigerated transport and cold storage. As such, three separate computational models (Figure 5) are constructed. For precooling and refrigerated storage, air ventilates the pallet horizontally (Figure 5a), whereas for refrigerated container transport, air ventilates the pallet vertically (Figure 5b). The inlet and outlet sections are chosen long enough to avoid an impact of these boundary conditions on the airflow and heat transfer in the pallet. The length of the inlet and outlet section is 0.4 m and 1.6 m, respectively. The inlet and outlet could be located relatively close to the pallet because a large pressure drop is created over the pallet. To avoid highly skewed grid cells (control volumes) near the point of contact between two fruit during mesh generation, a gap of about 3 mm is

left between adjacent fruit. This was found to lead to the most stable numerical solution, whereas point contact or small overlaps between the fruit provided unstable solutions in some cases.

Meshing of the computational models was done using tetrahedral cells with about 40 million tetrahedral cells for each model. Tetrahedral control volumes are placed on the inside and outside surfaces of the fruit. The wall y^+ is smaller than 185, 6 and 3 for precooling, refrigerated transport and cold storage, respectively. The spatial discretization error was quantified via a mesh dependency study combined with Richardson extrapolation. It is 2.5% for mass flow rates in the box and 5% for convective heat transfer coefficients on the fruit surface.

On the outlet, the imposed airflow rate is a uniform air speed. Its value depends on the specific cold chain unit operation. The airflow rates (see Table 2) in the present study are 0.2, 0.02 and 0.002 L s^{-1} kg^{-1} of fruit for precooling, transport and storage. These flow rates are chosen to be representative of the current commercial practice. Note that these flow rates differ a factor 10 from one another. Note that this implies that for the Opentop packaging, which has a lower packing density per pallet (3900 fruit instead of 5120 for Standard and Supervent), the speed is slightly lower than for the other packaging (Table 2). This effect is counteracted in part by the fact that Opentop pallets are cooled along their short side, in comparison to Standard and Supervent pallets. This, in turn, reduces the total inlet surface area which increases the speed for a certain flow rate. At the inlet, the atmospheric pressure is imposed with a low turbulence intensity of 0.1%. The air temperature at the inlet, or the so-called delivery-air temperature, is different for each evaluated supply chain scenarios (see Table 2).

The lateral boundaries of the extended inlet and outlet sections and the vent openings on the lateral carton surfaces of the complete pallet are specified as a symmetry boundary condition. This choice assumes that every single pallet has another adjacent pallet. This idealized assumption does not account for possible gaps

between the pallets, which can be present in reality. The impact of such gaps was investigated by numerical simulations recently (Defraeye, Cronjé, Verboven, Opara, & Nicolai, 2015). Although such gaps are blocked as much as possible with void plugs in practice, they can still be present sometimes, and can form preferential pathways between pallets. The size and location of such gaps are however very difficult to predict or quantify and can differ between different shipments. In this study, the impact of possible gaps between pallets was not included as a design parameter. No-slip surfaces with zero roughness are used for carton surfaces and fruit surfaces.

2.4. Numerical simulation

The simulations are performed with the open source CFD code OpenFOAM 2.4.0. The Reynolds-averaged Navier-Stokes (RANS) equations with the shear-stress transport k-ω turbulence model (Menter, 1994) are used to solve for turbulent flow. A turbulence model was used since even at low speeds, high airspeeds, so turbulent flow, can occur near the vent holes. Wall functions are applied to solve airflow and heat exchange in the boundary layer near the fruit and carton surfaces. The applied wall functions switch automatically from a standard wall function approach to a low-Reynolds number formulation, based on the grid density in the boundary layer. This switching takes place around a y^+ value of 11, using a blending function between the viscous and logarithmic region. In this way, the wall functions have a wide range of y^+ values in which they are applicable, and can be accurately used for both low- and high-Reynolds number turbulent flows. The accuracy of the shear-stress transport turbulence model combined with wall functions to model the boundary layer was validated already by the authors and co-workers on several occasions (Ambaw et al., 2012; Defraeye et al., 2013; Delele et al., 2009) for the same turbulence model and a similar geometrical model as used in the present study. All the details of the validation procedures can be found there. The agreement between CFD

and experiments was satisfactory. As an example, for Supervent packages, the differences in seven-eighths cooling time were below 5%. The initial temperature of cartons and the fruit was 21 °C. The thermal properties of the fruit are a density of 960 kg m^{-3}, thermal conductivity of 0.386 W $m^{-1}K^{-1}$ and specific heat capacity of 3850 J $kg^{-1}K^{-1}$ (Wu et al., 2018; Wu & Defraeye, 2018). A time step of 60 s was used, as determined from a sensitivity analysis. First, the steady airflow field is calculated for every unit operation. In the next step, the transient heat conservation equation is solved in the air and fruit domain. Thereby, the air and fruit temperature profiles are obtained throughout the complete cold chain. As the airflow was steady over time (as no buoyancy was modeled), the airflow field did not need to be recomputed anymore during the transient simulations. This removed the need for solving the airflow conservation equations during the transient cooling process. As such, the computational cost was reduced a lot (Wu et al., 2018; Wu & Defraeye, 2018). The two-step approach is often applied for forced-air cooling applications.

Not accounting for buoyancy essentially means that no temperature-driven density difference flow is modeled, so only forced-convective flow is considered. In addition, this implies that the temperature does not influence the flow field, by which heat can be considered as a passive scalar. As mentioned, this assumption simplifies the solution procedure a lot and reduces the computational cost. Especially at very lower airspeeds, such as in storage rooms, and at the start of the cooling process, when temperature differences in the air are larger, buoyancy could however contribute. Investigating the impact of buoyancy in such cases is definitely a topic of further research, but will pose challenges to numerical stability, convergence and computational cost. For this reason, it is very rarely taken into account in CFD studies in postharvest engineering.

The advection terms are discretized by the second-order upwind scheme. The time derivative is discretized by the first-order, bounded, implicit Euler scheme. The SIMPLE algorithm and merged PISO-SIMPLE (PIMPLE) algorithm are adopted for velocity-pressure coupling for steady state and transient simulations, respectively. Further details on the numerical modeling approach, model assumptions, solution method and discretization

approach can be found in (Wu et al., 2018; Wu & Defraeye, 2018), including on the other physics that are included.

2.5. Kinetic rate-law quality model

A kinetic rate-law model for fruit quality evolution was presented previously (Wu et al., 2018; Wu & Defraeye, 2018), so only the main aspects are highlighted here. This simple model quantifies the change in overall fruit quality, indicated by parameter *A*, based on a kinetic rate law (Robertson, 2016; Van Boekel, 2008):

$$-\frac{dA}{dt} = kA^n \quad (1)$$

with t the time [s], k the rate constant [s^{-1}], n the order of a reaction. We assume a zero-order reaction here for the change of the overall quality *A*. This means that the temporal change of *A* for a specified temperature is a line, where the slope is linked to the magnitude of *k*. An example of a zero-order reaction is enzymatic degradation (Robertson, 2016; Van Boekel, 2008). First-order reaction (such as vitamin loss), can also be modeled similarly.

The rate constant *k* quantifies the temperature relationship of the fruit quality loss (Robertson, 1993):

$$k(T) = k_0 e^{\frac{-E_a}{RT}} \quad (2)$$

where k_0 is a constant [d^{-1}], E_a is the activation energy [J mol^{-1}], R is the ideal gas constant (8.314 J mol^{-1} K^{-1}), T is the absolute temperature [K]. The constant k_0 and E_a are inferred from quality decay data.

This model was calibrated based on following assumptions, stemming from experimental data: citrus fruit can be stored for approximately 56 d at 4 °C (Cantwell, 2001) where a rise in temperature of 10 °C from a certain temperature halves the storage life. As such, if the fruit is kept 56 d hours at 4 °C, the entire quality, and

thereby also the fruit, is assumed to be lost, so A(56 d, 4 °C) = 0%. As such, E_a and k_0 were determined to be 4.59×10^4 J mol^{-1} and 7.89×10^6 d^{-1}, respectively. After calibrating this quality model, the temperature-dependent evolution of this fruit quality of every single fruit was predicted throughout the cold supply chain. The temperature used to calculate the quality evolution can be for example the core temperature or the average fruit temperature. In this study, the fruit core temperature was used to derive the quality evolution of every single fruit. This choice is conservative as the fruit core is typically the last location that reaches the target temperature.

2.6. Different cold chains

Three cold chain scenarios (see Table 2) are assessed for their impact on the cooling of a pallet of fruit. These are currently employed as postharvest supply chain strategies in the citrus fruit industry in South Africa.

The "forced-airflow precooling" chain includes cooling (3 d to 3 °C), refrigerated transport at cold-disinfestation temperatures for pests (24 d to -1 °C) and subsequent cold storage (14 d to 4 °C). This chain implies rapid removal of the bulk of the stored heat by precooling, followed by further removal during refrigerated transport. The next cold chain "ambient cooling" does not include forced-airflow cooling. Alternatively, fruit are kept in standard cold storage for 5 d to 3 °C, before shipment, so slow cooling. This strategy is often named static cooling in the citrus industry. Following that, fruit are loaded in a refrigerated container for transport (24 d to -1 °C) and subsequent cold storage (14 d to 4 °C) after shipment. In the third cold chain, "ambient loading" (Defraeye, Verboven, Opara, Nicolai, & Cronjé, 2015), fruit are loaded directly into the container after packaging. Following 24 d at -1 °C, fruit are stored for 14 d in 4 °C. Ambient loading is applied in South Africa to reduce the cold chain length and to enable cooling after harvest in areas where there are insufficient facilities to precool.

2.7. Evaluation of cooling rate

The fruit's cooling rate is quantified by its temperature-time history. This is measured in the center core of each citrus fruit. From these core temperature profiles (T [K]) the dimensionless temperature change (Y) was calculated.

$$Y = \frac{T - T_a}{T_i - T_a} \tag{3}$$

where subscripts *i* and *a* imply the initial fruit temperature and the air's delivery temperature in the cold chain unit operations, respectively. From Y, the seven-eighths cooling (or heating) time (SECT, $t_{7/8}$) was calculated. The $t_{7/8}$ is the time required to bring the temperature difference between initial-fruit and delivery-air temperature down by seven eighths (Y=0.125). The SECT is a useful parameter to characterize the cooling behavior of the fruit in each of the unit operations.

3. Results and discussion

3.1. Cooling kinetics of individual unit operations

The cooling behavior is evaluated separately for each unit operation to quantify how large the differences between the three package designs are. The fruit core temperature is used here for calculating the SECT of every single fruit. The reason is that the core temperature is typically the last location that reaches the target temperature. For this reason, it is measured in commercial cooling operations, and especially in cold treatment protocols, for monitoring the cooling process by inserting a temperature point probe. The use of this temperature to assess fruit cooling is thereby the most conservative scenario.

In Figure 6, the SECT is depicted for all unit operations and packaging by showing the average value and

standard deviation over all fruit in the pallet. Here, all fruit are cooled down completely to the delivery-air temperature within one unit operation. These SECT data of all the fruit in the pallet are also presented in Figure 7, but now grouped and averaged per vertical column for each separate carton (C01-C10, for precooling and storage so horizontal airflow) or per horizontal layer (L1-L13) (for transport so vertical airflow). Next, to the average values per column and layer, the standard deviations are also shown. In Figure 8, the SECT per box is represented for all unit operations and packaging.

Precooling

The Standard and Supervent packaging cool similar, which is in agreement with previous studies of the authors for a smaller computational model, with a slightly different computational model build-up (Defraeye et al., 2014). At the currently evaluated flow rates (0.2 L s^{-1} kg^{-1}), the Standard packaging cools slightly faster, when averaged over the pallet. For both packagings, the more upstream the box is, the faster it cools, although the flow rates through each row of boxes is the same due to the conservation of mass, i.e. all air which enters the pallet also leaves. One reason is that the downstream boxes are exposed to higher air temperatures as heat is added to the flow from the fruit upstream, by which the fruit more downstream will cool slower. This principle is also valid for other packaging and other unit operations. Also, the blockage of the vent holes for Standard and Supervent packages induces a high SECT for cartons C08 and C09, which are double or triple than those of the upstream boxes (C01-C03).

The Opentop packaging cools slower and also more heterogeneously than the other two. This is counter-intuitive at first as Opentop cartons have the largest open area of vent openings on both its long and short side of the packaging (Table 1). This is due to:

- The difference in TOA between the long and short side of the package. First, this creates a difference in aerodynamic resistances, by which the preferential pathway will be through C03-C05 instead of C01-C02, leading to higher speeds there, which can be seen from Figure 9b. Also, the cooling air accesses more easily most of the fruit in C03-C05 since the ventilation opening is wider. An additional reason is that the path length for airflow is longer for C01. As such, the air is heated up more at the point when it reaches the fruits at the back of the package, by which fruit cooling in these packages is slowed down.
- The configuration of the vent openings on the short and long sides of each box. Since they are not distributed that homogeneously compared to the other two packages, but mainly have large openings at the top, the cooling air is directed primarily over the top layer of fruit. As such, the access of the air to the bottom layer of fruit in each box is more difficult. As such, this bottom layer was also found to cool slower than the top layer, inducing an additional cooling heterogeneity. On average, the bottom layer cooled less than 5% slower than the top layer (based on the SECT). However, individual differences in SECT of over 50% are found between fruit in the bottom and top layer.
- The airflow rate (0.2 L s^{-1} kg^{-1}) results in a slightly lower speed in the Opentop packaging, due to the lower packing density (Table 2). Also, the maximal speeds (Figure 9) are lower as less flow acceleration occurs near the vent openings, due to the large total open area (Table 1).

Although no blockage of vent openings is present with the Opentop packaging, some upstream boxes still cool more than twice as fast as the downstream ones. This limited performance of the Opentop packaging contradicts the experimental study of (Wu, Häller, Cronje, & Defraeye, 2018), which found a better performance for the Opentop packaging for precooling. There are several reasons that can be attributed for these differences. The experiments were conducted on a commercial precooling facility. As such, the airflow rate through the different packages could not be controlled, as this was the result of the cooling infrastructure

and the pressure resistance of the pallets. As such the airflow rates differed for Supervent and Opentop. In the current computational study, similar airflow rates were imposed for both Supervent and Opentop. This makes a comparison between both studies difficult. The computational study shows however that at a similar airflow rate, the Supervent packaging seems to cool better than Opentop packaging. Also, note that the fruit size and packing density differed in both studies. **Refrigerated transport**

The Supervent packaging cools faster than the other two packagings. This is mainly attributed to the specific vent hole configuration, where vent openings are positioned along the side edges of the packaging. As such, vertical ventilation channels of cold air are formed, which can be seen from Figure 9a. Combined with the central opening at the bottom and top, a very uniform distribution of the cooling air through the package is achieved. Opentop packaging has very small ventilation openings by which locally very high speeds are generated, which can be seen from Figure 9a. The access of the cold air to the rest of the fruit is limited and also the airflow distribution is much less uniform. All packages cool progressively slower towards the top of the pallet, and this occurs in a quite linear manner.

Cold storage

The Supervent packaging cools faster than the other two packagings. A lot of similar observations can be made as for precooling, for example, the SECT distribution between the different boxes. The main reason is that the airflow direction is the same, but only the airflow rate differs. At low airflow rates (cold storage) the fruit have a less uniform temperature reduction than at high airflow rates (precooling) for Standard and Supervent, but this is not found for Opentop which cools similarly uniform (but not similarly fast) in both unit operations. The Standard packaging however cools much slower than the other two, where for precooling it cooled the fastest. This is an interesting observation, particularly since the Opentop pallet contains 24 % less fruit, and is subjected to slightly lower airspeed.

A first reason to explain this observation is that at different airspeeds, a different velocity distribution is found in the pallet for each packaging, which can be seen from the streamlines for precooling and storage for Opentop (Figure 9). This will thereby also induce a difference in the cooling of the individual fruit in the packaging for the different unit operations. For Opentop, for example the cold airflow penetrates the stacked fruit inside the packaging better at low airspeeds, which induces better access of the cooling air to the bottom layer of fruit. This reduces the heterogeneity between the bottom and top layer of fruit. At high speeds (precooling) on the other hand, the fast flowing horizontal air only accesses the top fruit and does not cool the lower fruit on the bottom layers. As such, Opentop packaging seems to cool the two layers more efficiently, in a relative way, at lower air speeds.

A second reason is that at lower airspeeds, the air is able to extract more heat (relatively) as it passes over the fruit in the first packages (e.g. C01-C03), after which the air temperature also rises more during cold storage when passing the different boxes. As such, for cold storage, the boxes more downstream on the pallet will cool (relatively) slower than those upstream, compared to forced-air cooling. This increased heterogeneity for cold storage, compared to precooling, can clearly be seen in Figure 8, and is especially pronounced for the Standard package. As a third reason, the cartons C08 and C09 seem to cool even slower during storage, which could indicate that the cooling air penetrates these two boxes at even further reduced airspeeds.

Summary

Throughout all unit operations, Supervent outperforms the other packages, by which it can be considered the fastest and most uniformly cooling package. This is attributed to the specific vent hole configuration, where the vent holes are positioned along the side edges of the packaging. This enables the vent holes to form ventilation channels of cold air for both vertical and horizontal flow. The superior performance of Supervent

was identified before, but for smaller entities of fruit (Defraeye, Cronjé, Verboven, et al., 2015; Defraeye et al., 2013). For all boxes, the spatial heterogeneity in cooling behavior inside the pallet is very apparent for different unit operations, where precooling provides the most uniform cooling. This heterogeneity will directly affect fruit quality and shelf life as well, as illustrated in the next section. It needs to be mentioned that all packages were evaluated at similar airflow rates (Table 2). In reality, the resistance to airflow of the palletized package and the resulting pressure drop over the pallet will also determine the resulting air speed (Defraeye et al., 2014).

3.2. Cooling kinetics and quality evolution of complete cold chain scenarios

By combining subsequent unit operations into a cold chain, three different cold chain scenarios are simulated (Table 2). In Figure 10, their thermal history is given for all packaging designs, as presented by the volume-averaged temperature of all fruit inside the pallet. This implies as well that the volume-averaged temperature of each fruit is used, so averaging is not done based on core temperature. It is clear that the forced-airflow precooling scenario provides the fastest cooling. Ambient cooling (static cooling) only reduces the fruit temperature very slowly, by which the fruit still did not reach the set point temperature at the time of loading into the refrigerated container for transport. The differences between the packages are relatively limited, but show an inferior performance for the Opentop packages.

Using this thermal history, the quality evolution of the fruit in the pallet is calculated for several cold chain

scenarios for each packaging design. The fruit core temperature is used to derive the quality evolution of every single fruit. In Figure 11, the evolution in the quality of every single fruit in two different boxes (shown in Figure 3) is shown for the three package designs and the three scenarios. The remaining end quality is given as the percentage of initial quality (A_{ini}=100%), and the fruit is considered lost if all quality is gone (A_{end}=0%). These two different boxes are chosen in that way that they are exposed to the most extreme (high and low) approach flow air temperatures. To this end, one box (Box03) is always located upstream, so at the cold air inflow side, and one box is located downstream (Box 62 for Opentop and Box 79 for the other two packages) for precooling, transport and storage. The aim is to improve the quantification of the heterogeneity in the quality evolution within a pallet, which originated from the temperature heterogeneity (Figure 8).

The forced-airflow precooling and ambient loading cold chain have a quite homogeneous quality evolution. On average over the entire pallet (results not reported), very similar values are found, despite the clear differences in cooling behavior (Figure 10). The rather limited differences between the two protocols are attributed to the timescales for fruit quality decay, which are much larger than those for cooling. As such, a faster cooling via precooling in the first few days, compared to cooling inside the container, does not lead to significant differences in the quality loss, which occurs much slower. Note however that since the ambient loading scenario has a shorter duration, its end quality is even higher than for the forced-airflow precooling chain. The logistical advantage of saving time before shipment by ambient loading takes the upper hand over cooling faster. Note that the quality variation within the pallet (box 03 vs. box 79 or 62) is however larger for ambient loading. The ambient cooling chain, on the other hand, induces a much larger quality loss. This is directly linked to the prolonged storage with much slower cooling rates, and the resulting more elevated fruit temperatures before shipment. The differences between packaging designs are quite limited, which is again related to the different timescales in cooling and quality decay. Opentop exhibits a slightly lower quality as it had the overall worst cooling behavior over most unit operations (Figure 6).

3.3. Cooling kinetics of different stacking patterns

The impact of the stacking pattern (Figure 4) on the cooling kinetics is evaluated in Figure 12. The averaged seven-eighths cooling time for each box, scaled with the average SECT for that pallet for that unit operation, namely $SECT_{avg}$, is shown for the Supervent packaging for three unit operations for regular and staggered stacking. The stacking pattern significantly affects the cooling heterogeneity within the pallet for each unit operation. As expected, for vertical airflow, this leads to a higher heterogeneity within the pallet (vertical direction) but also within a certain layer of boxes. In addition, for precooling and storage, the staggered stacking leads to a very inefficient cooling of the boxes C08 and C09 in the bottom layer. In stacking cartons on a pallet, there will be a tradeoff between mechanical stability and achieving uniform cooling of the pallet throughout the cold chain. As such, apart from the individual package design, their pallet stacking plays a role concerning vent-hole blockage.

4. Conclusions

This pioneering study unveiled how ventilated packaging design and cold chain scenarios affect the cooling kinetics and fruit quality evolution for each of the thousands of fruit packed inside a pallet. Concerning the three evaluated packaging designs, the Supervent package outperformed the others by providing overall the fastest and most uniform (homogeneous) cooling. This is attributed to the formation of aligned ventilation pathways via the lateral vent holes. The performance of the Standard package was very similar during forced airflow cooling, but at lower speeds, more inefficient cooling was observed. The Opentop packaging exhibited rather high and non-uniform fruit cooling times. The main causes were the unequal distribution of the vent openings on the long and short sides, creating preferential pathways, and the fact that these openings were located at the top of the package, so inducing preferential cooling of the top layer of fruit. Concerning the cold chain scenarios, forced-airflow precooling was able to bring down the fruit pulp temperature the fastest after harvest. Ambient loading, where “warm” fruit are loaded at ambient temperatures in the container, proved to be a promising alternative. Despite its slightly slower cooling, it provides a logistical advantage of saving time by direct loading the cargo in the container. This shorter cold chain also resulted in a higher final product quality. The ambient cooling scenario, where fruit are stored in a cold store before loading in the container, is not advised as it induces much higher quality losses. Finally it was shown that the stacking of the pallet in a mechanically more stable way negatively affected the cooling heterogeneity, due to blockage of the vent holes.

By applying our recently developed virtual cold chain methodology for such large ensembles of fruit, we could obtain essential insights, which were not visible before on smaller computational models. We were able, amongst others, to identify for a certain cold chain, which specific box on the pallet the customer should choose to have the longest shelf life, or also which box the retailer should sell first. Such results can be very

475 useful for logistics planning as well.

476 Finally, the obtained data on cooling and quality evolution of individual fruit, and the role of packaging, can be
477 incorporated in life-cycle assessment. Thereby, data gaps in LCA can be closed successfully by providing more
478 accurate data on cold-chain energy use for fruit, compared to what is available, for multiple packaging
479 options.

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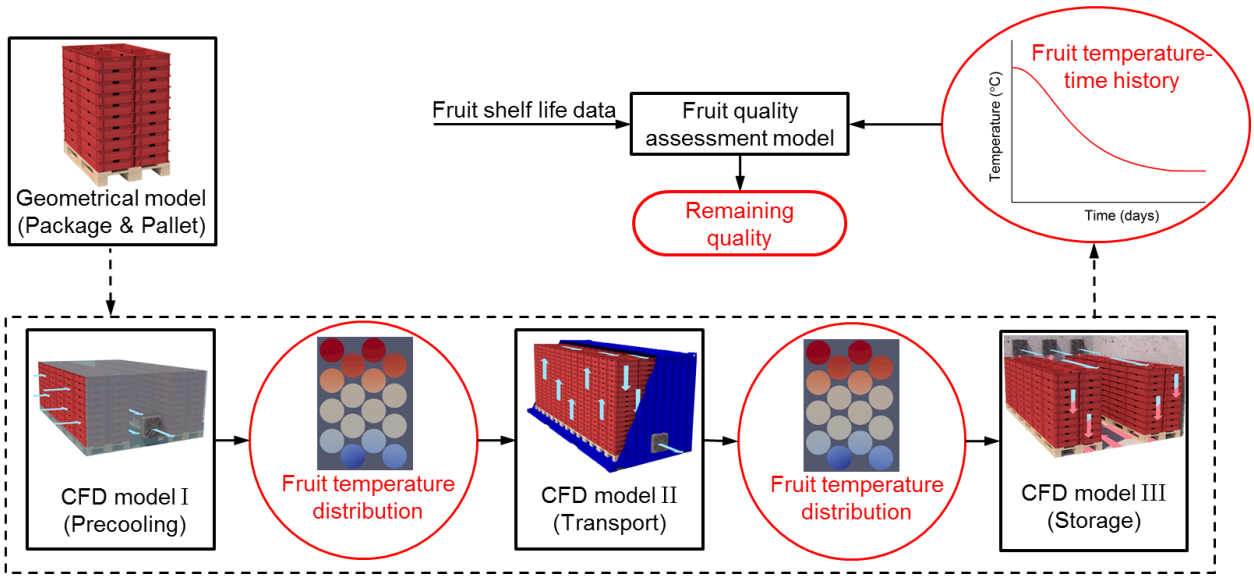


Figure 1. The Virtual Cold Chain (VCC) method illustrated by a typical cold chain consisting of precooling, refrigerated transport and cold storage (reproduced with permission from (Wentao Wu et al., 2018)).

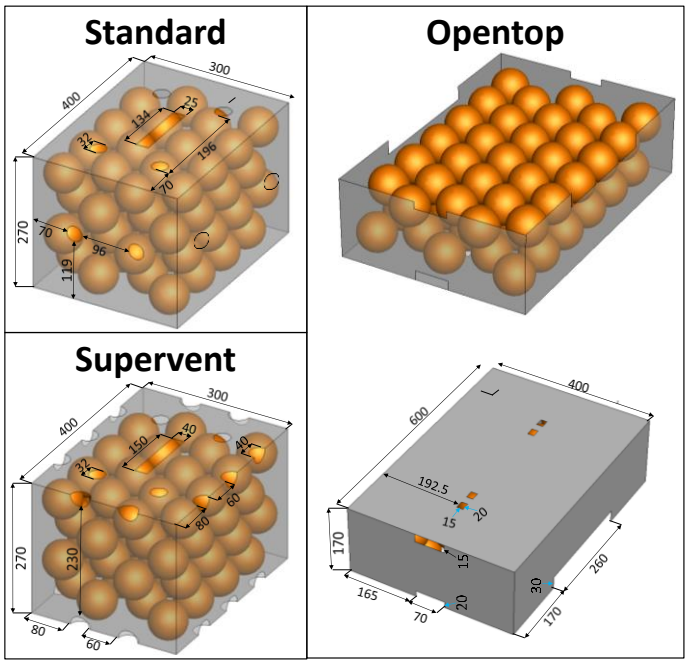


Figure 2. Geometry and dimensions of the Standard, Supervent and Opentop carton (view from the top and bottom), packed with orange fruit.

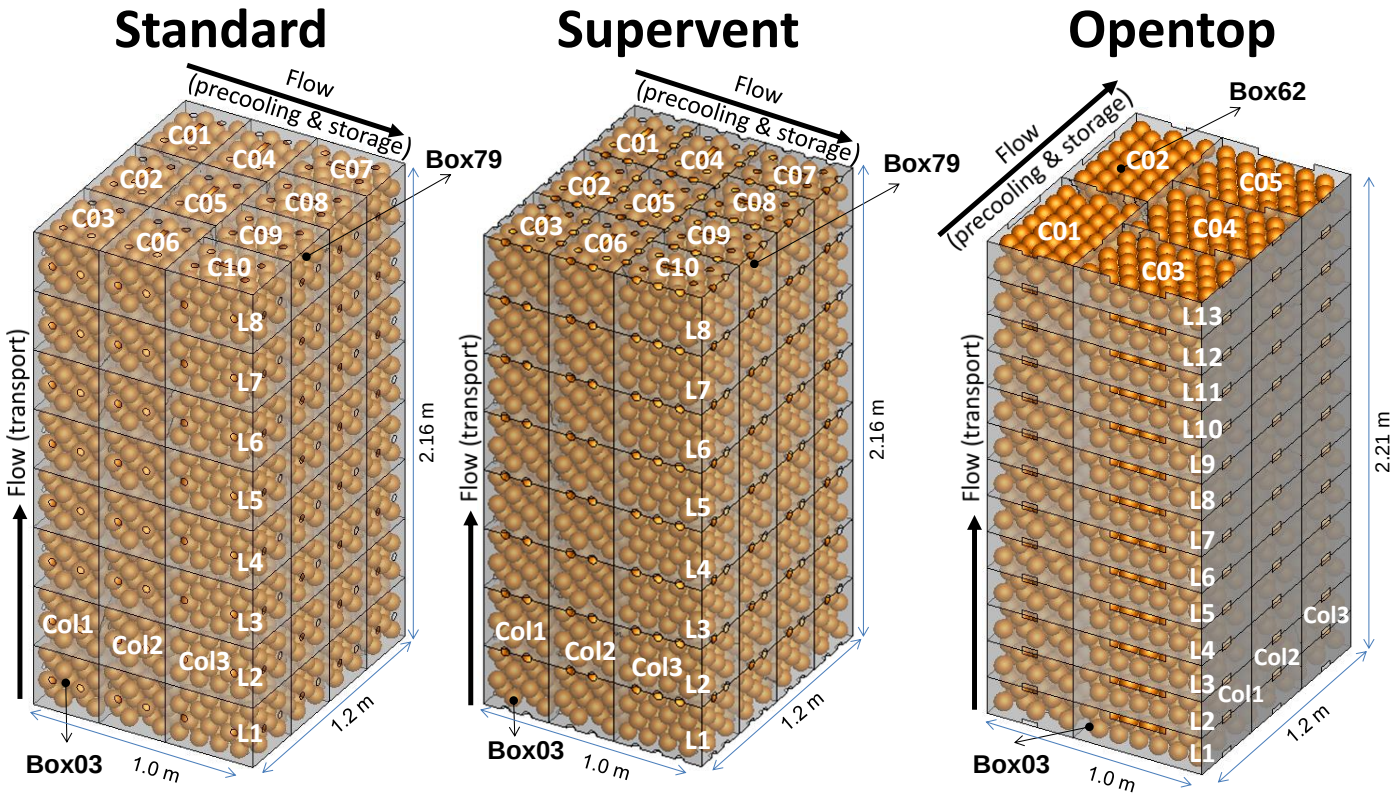


Figure 3. High-cube citrus pallet of the Standard, Supervent and Opentop carton, stacked in different layers.

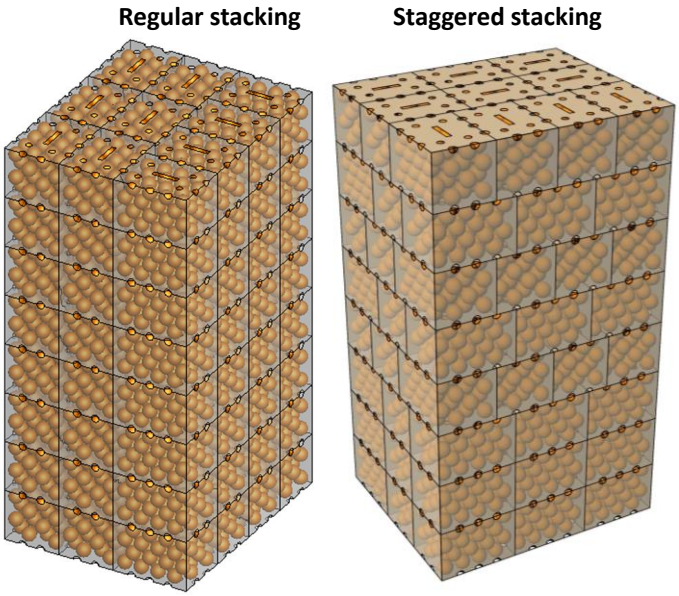
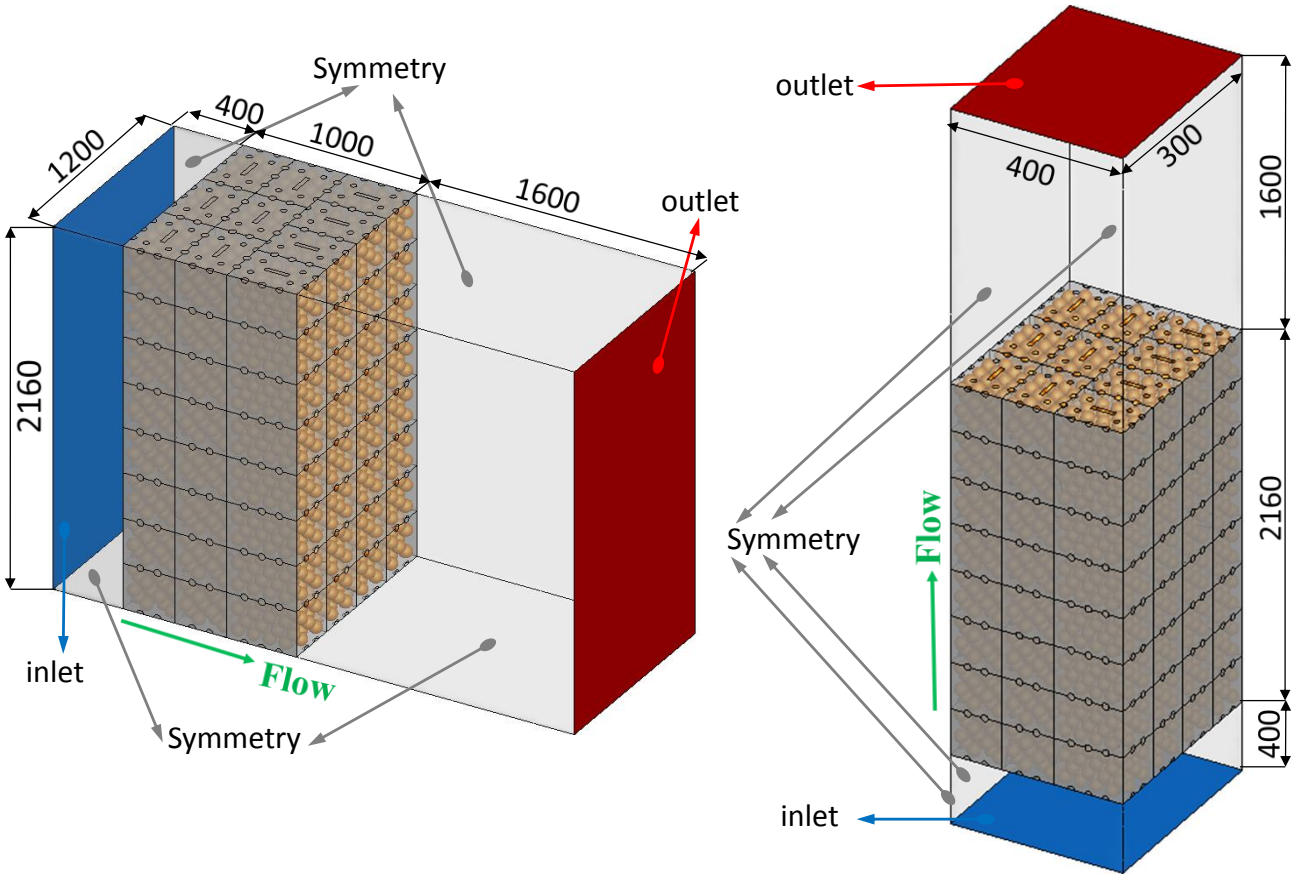


Figure 4. High-cube citrus pallet of the Supervent carton, according to a regular and a staggered stacking pattern.



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643 ***Figure 5. CFD models (with boundary conditions) for three unit operations, as illustrated for Supervent***

644 ***packaging: precooling, transport and refrigerated storage (units are in mm). Note that the pallet height is***

645 ***slightly different for Opentop packaging.***

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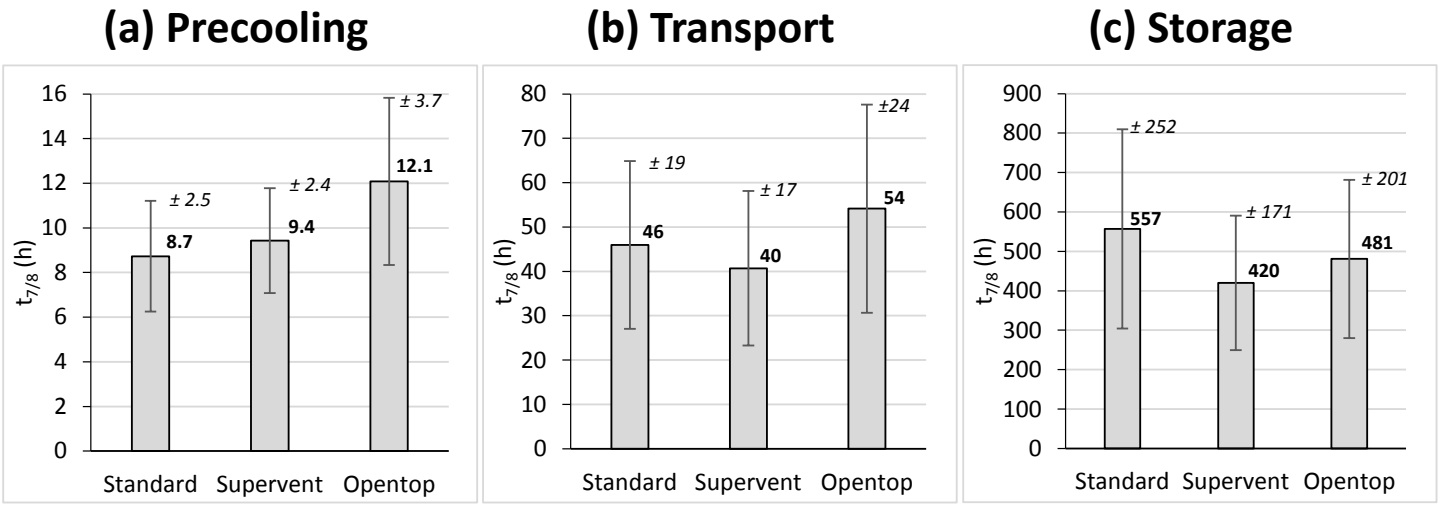


Figure 6. Seven-eighths cooling time of the fruit during precooling, refrigerated transport and refrigerated storage for three packaging: SECT averaged over an entire pallet of fruit and the standard deviation.

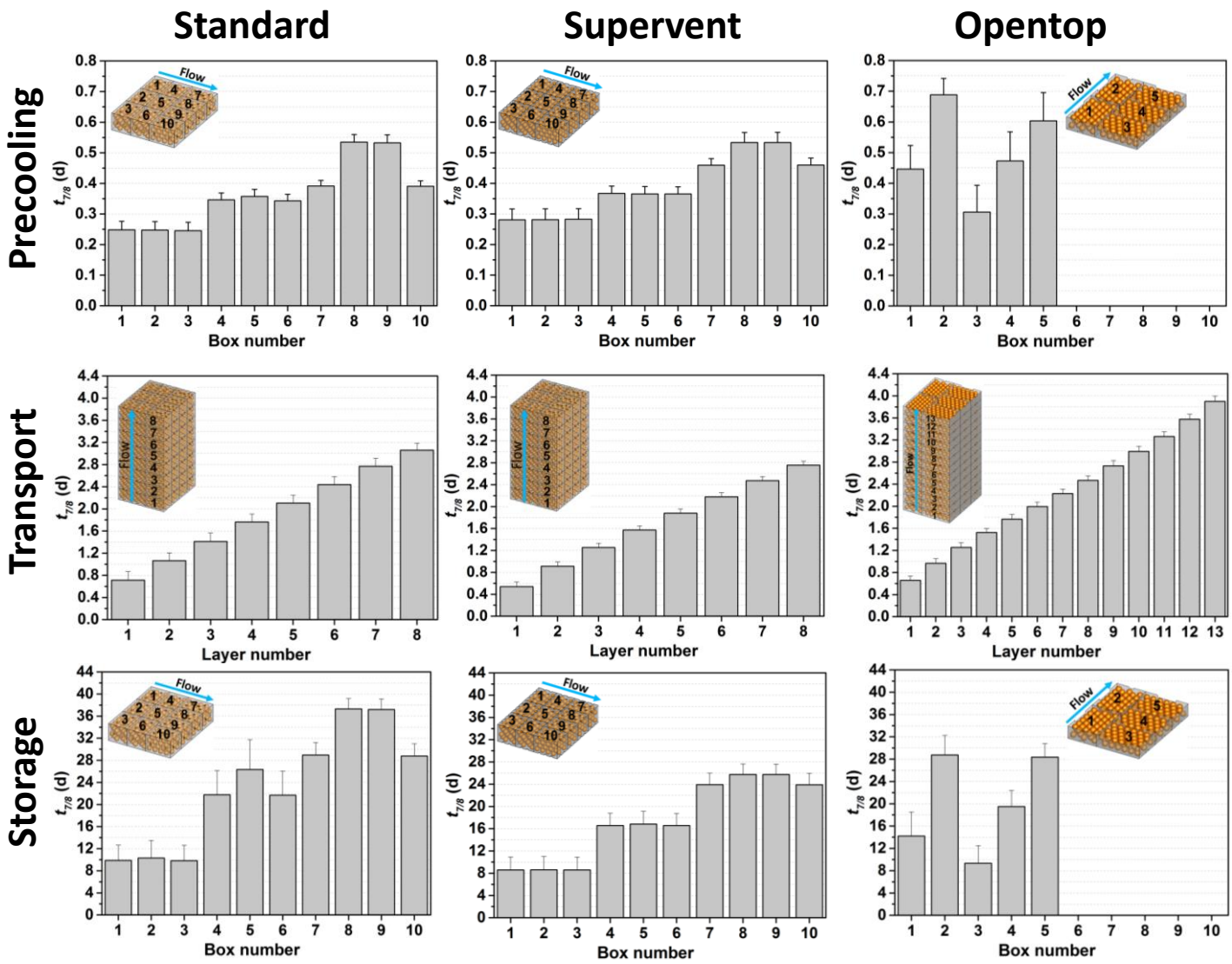


Figure 7. Seven-eighths cooling time ($t_{7/8}$) for each single box (C01-C10) for precooling and storage (averaged over all boxes in each vertical column and corresponding standard deviation), and for each horizontal layer of boxes (L1-L13) for transport (averaged value over all boxes in each layer and corresponding standard deviation).

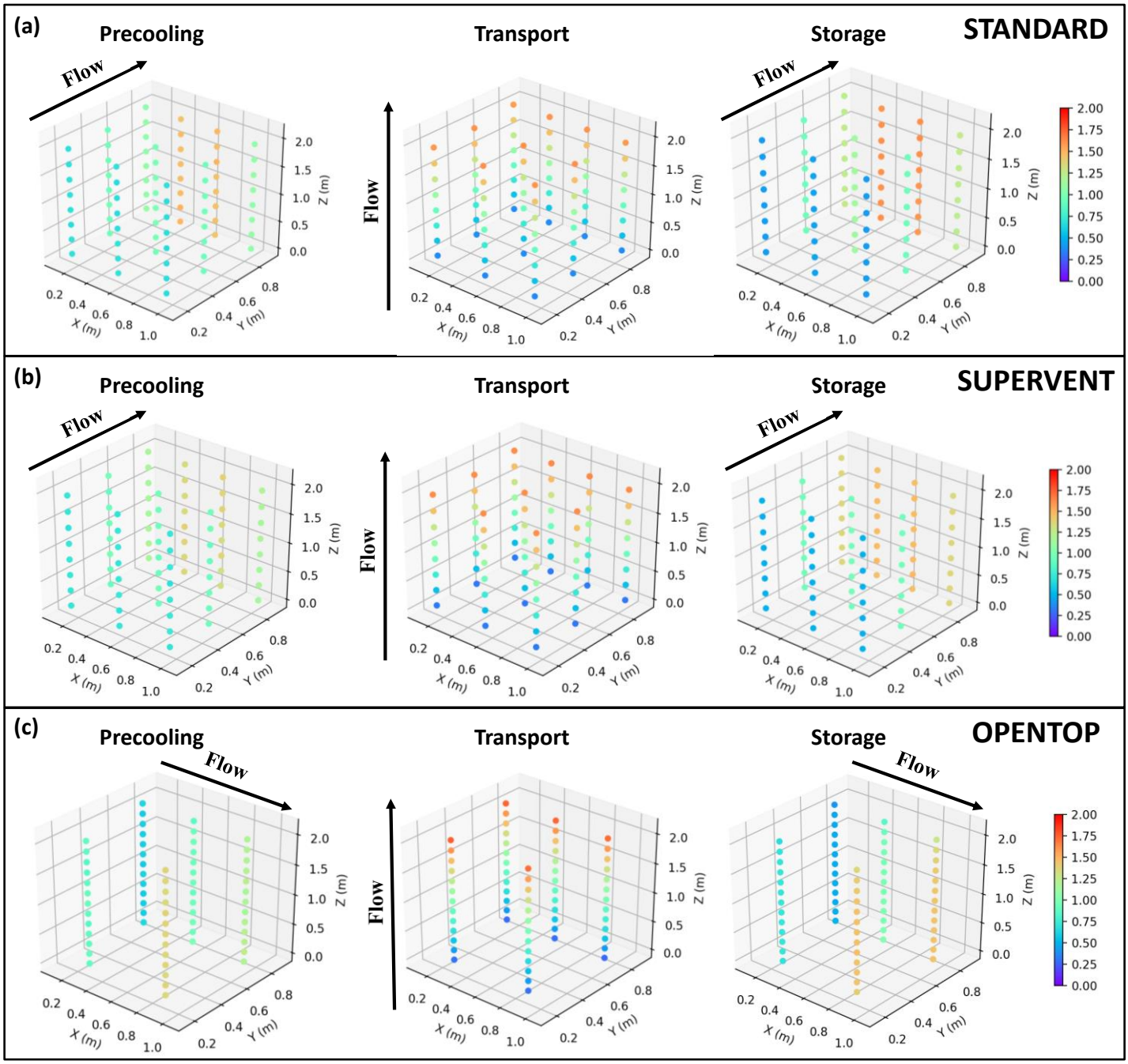
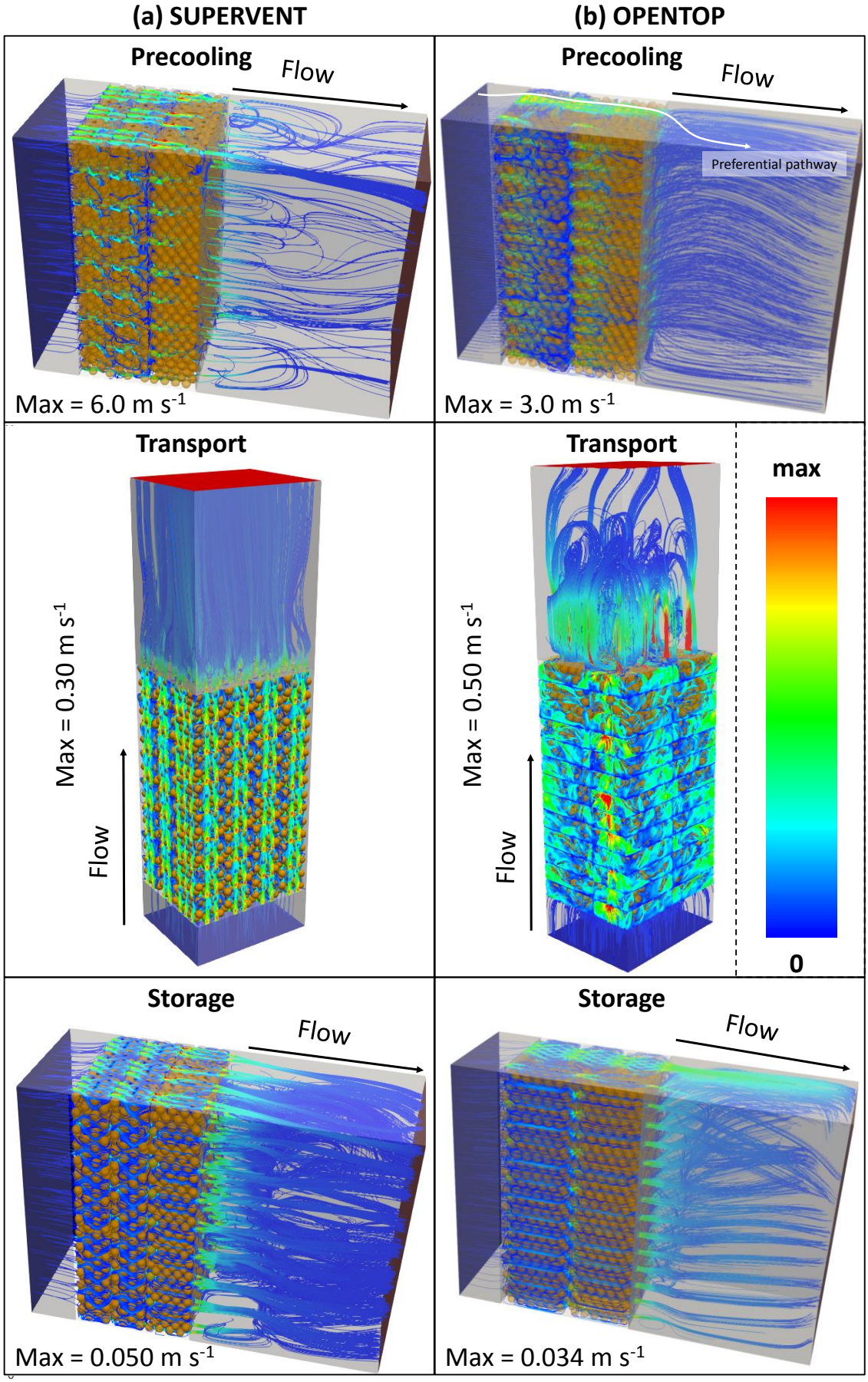


Figure 8. Seven-eighths cooling time for a pallet of Standard, Supervent and Opentop packaging for three unit operations (scaled with the average SECT for that pallet for that unit operation, namely $SECT_{avg}$), where each colored dot represents the averaged value of the $SECT/SECT_{avg}$ over a single box.


(a) SUPERVENT
(b) OPENTOP
Precooling
Flow
Max = 6.0 m s-1
Precooling
Flow
Preferential pathway
Max = 3.0 m s-1
Transport
Max = 0.30 m s-1
Flow
Transport
Max = 0.50 m s-1
Flow
max
0
Storage
Flow
Max = 0.050 m s-1
Storage
Flow
Max = 0.034 m s-1

661

Figure 9. Streamlines for a pallet of Supervent and Opentop packaging for three unit operations. The color bar is valid for each graph and the maximal values are indicated separately.

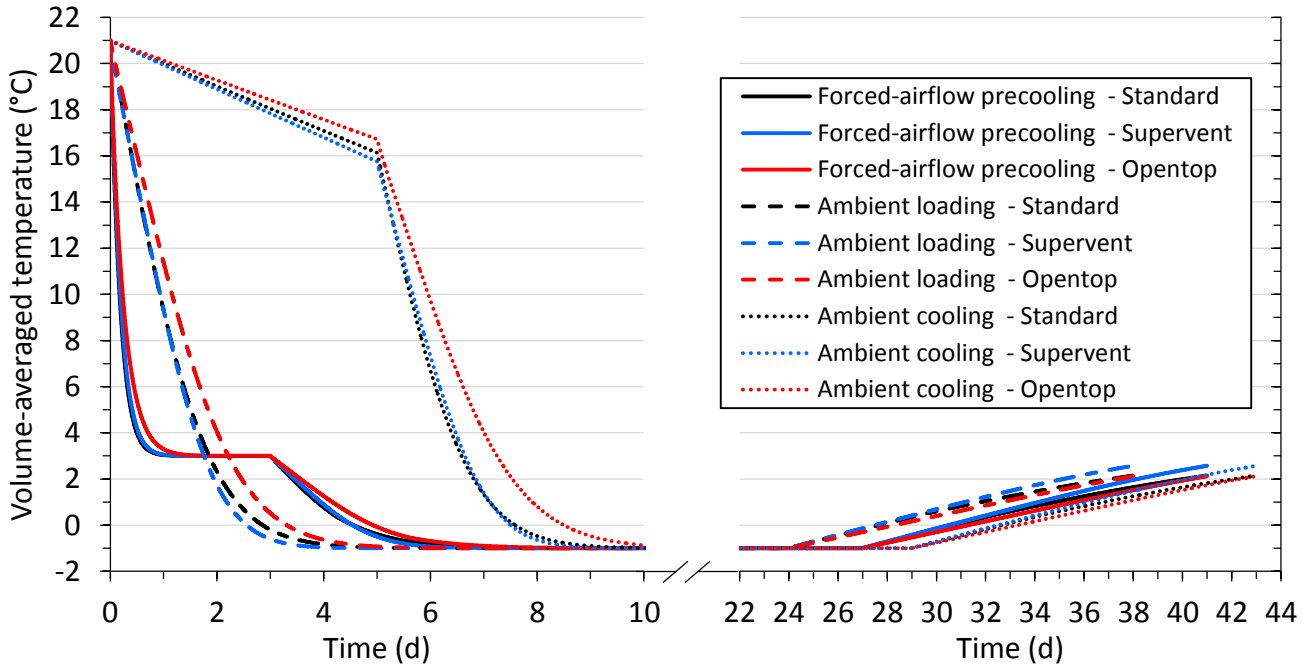
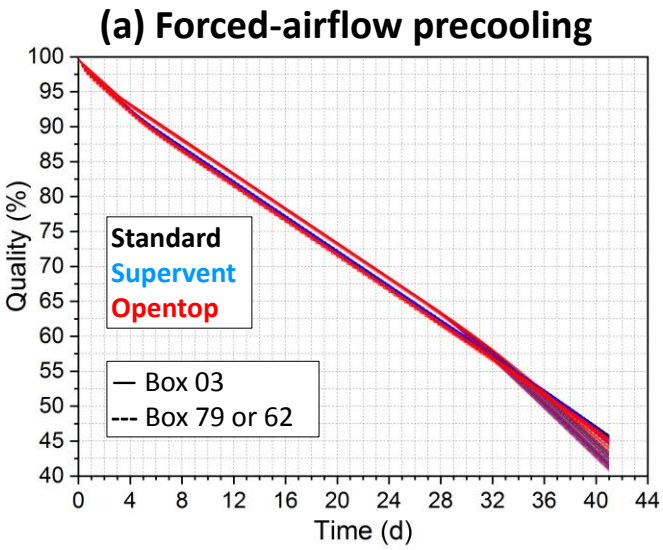
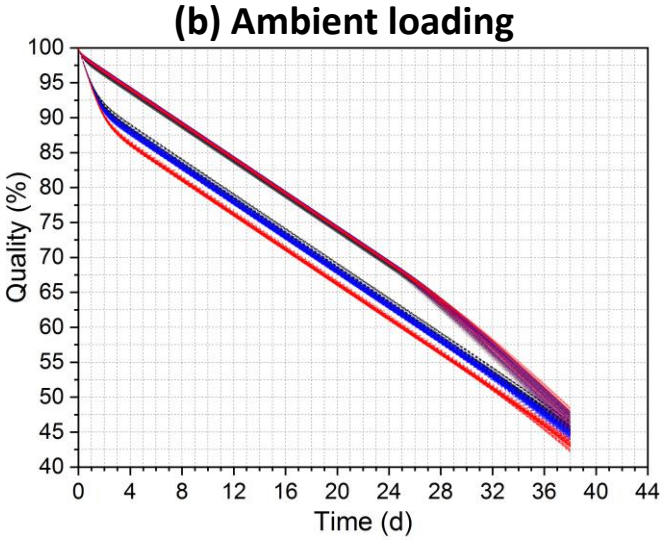
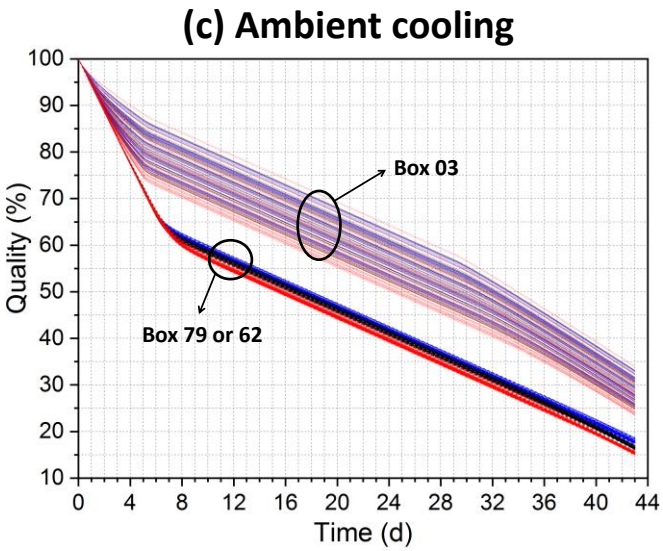


Figure 10. Volume-averaged temperature over all fruit in a pallet as a function of time in the three cold chain scenarios for all packaging designs.


(a) Forced-airflow precooling
Quality (%)
Time (d)
Standard
Supervent
Opentop
— Box 03
--- Box 79 or 62


(b) Ambient loading
Quality (%)
Time (d)


(c) Ambient cooling
Quality (%)
Time (d)
Box 03
Box 79 or 62

669

Figure 11. Quality evolution of individual fruit in Box03 and Box79 on a pallet with Standard (black lines) or Supervent (blue lines) cartons, and in Box03 and Box62 on a pallet with Opentop cartons (red lines) for the (a) forced-airflow cooling chain, (b) ambient loading chain, (c) ambient cooling chain.

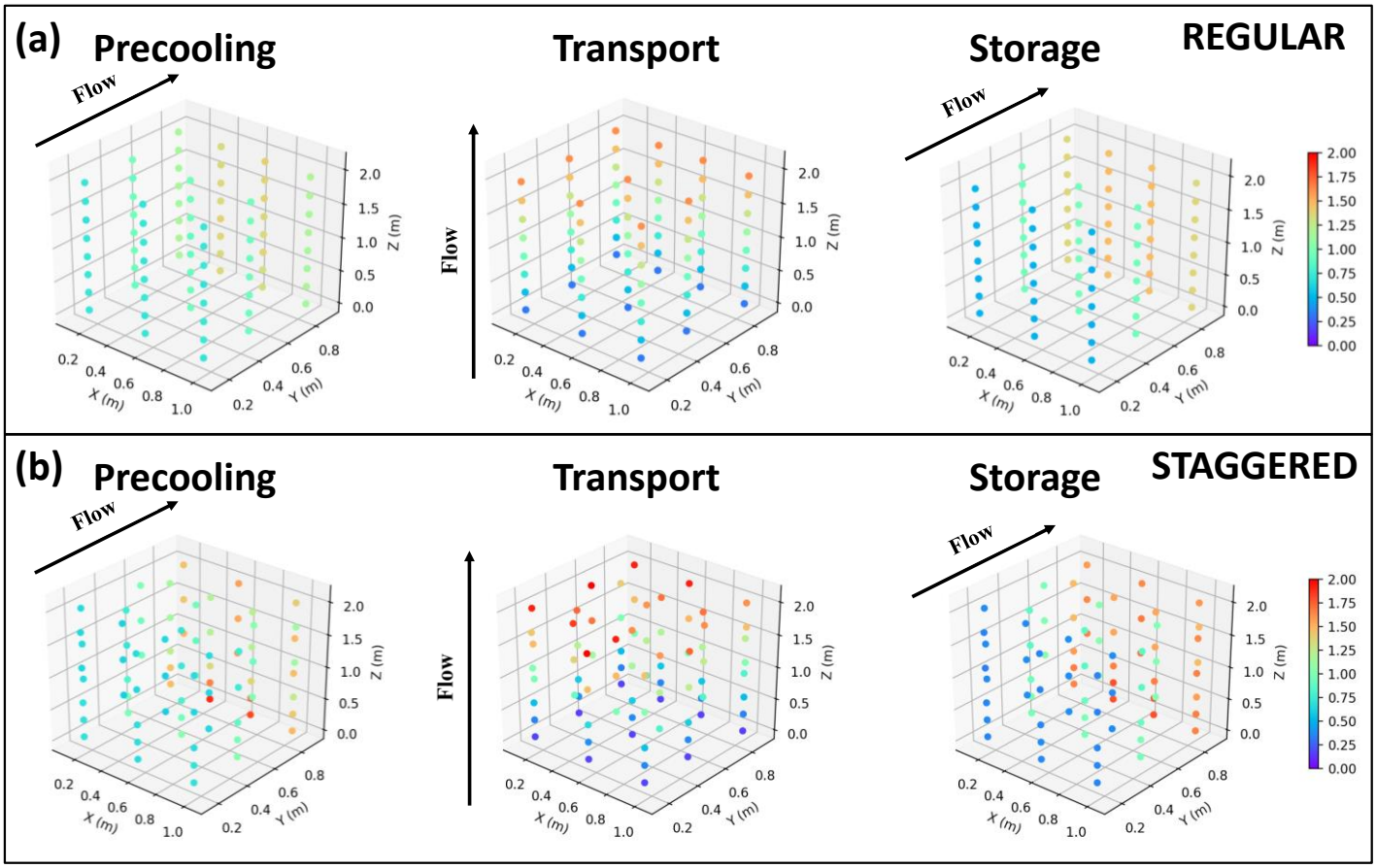


Figure 12. Seven-eighths cooling time for a pallet of Supervent packaging for three unit operations (scaled with the average SECT for that pallet for that unit operation, namely $SECT_{avg}$), for two different pallet stacking configurations (Figure 4): regular (results reported also in Figure 8) and staggered. Each colored dot represents the averaged value of the $SECT/SECT_{avg}$ over a single box.

Table 1. Total open area of the ventilation openings along the surfaces of each carton.

	Standard	Supervent	Opentop
Long side	1.5%	3.5%	7.6%
Short side	2.0%	3.1%	3.6%
Bottom	5.5%	10.7%	0.5%

Table 2. Boundary conditions for the different cold chain scenarios (a dash means that the cold chain does not contain the corresponding unit operation.).

Cold chain scenario	Precooling	Cold storage before shipment	Cold storage after shipment	Cold storage after shipment
Forced-airflow precooling	0.2 L $kg^{-1}s^{-1}$ 3 °C 3 days	-	0.02 L $kg^{-1}s^{-1}$ -1 °C 24 days	0.002 L $kg^{-1}s^{-1}$ 4 °C 14 days
Ambient cooling	-	0.002 L $kg^{-1}s^{-1}$ 3 °C 5 days	0.02 L $kg^{-1}s^{-1}$ -1 °C 24 days	0.002 L $kg^{-1}s^{-1}$ 4 °C 14 days
Ambient loading	-	-	0.02 L $kg^{-1}s^{-1}$ -1 °C 24 days	0.002 L $kg^{-1}s^{-1}$ 4 °C 14 days